

Formaldehyde-(14)C
3046-49-9 | DTXSID20184538

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 1.74

Global applicability domain: Inside

Local applicability domain index: 4.90e-01

Confidence level: 7.10e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>N,N-Dimethylformamide</div> <div>Measured: 7.94e-01</div> <div>Predicted: 1.12</div>	<div>Image not found</div> <div>1,4-Dioxane</div> <div>Measured: 5.01e-01</div> <div>Predicted: 1.06</div>	<div>Image not found</div> <div>Morpholine</div> <div>Measured: 2.82</div> <div>Predicted: 1.87</div>
<div>Image not found</div> <div>Furan</div> <div>Measured: 5.01</div> <div>Predicted: 4.88</div>	<div>Image not found</div> <div>Piperazine</div> <div>Measured: 3.89</div> <div>Predicted: 2.44</div>	